

# METHOD OF CALCULATING THE FREE ENERGY OF THREE-DIMENSIONAL ISING-LIKE SYSTEM IN AN EXTERNAL FIELD WITH THE USE OF THE $\rho^6$ MODEL

I.V. PYLYUK, M.P. KOZLOVSKII

*Institute for Condensed Matter Physics  
of the National Academy of Sciences of Ukraine,  
1 Svientsitskii Str., UA-79011 Lviv, Ukraine  
E-mail: piv@icmp.lviv.ua*

The microscopic approach to calculating the free energy of a three-dimensional Ising-like system in a homogeneous external field is developed in the higher non-Gaussian approximation (the  $\rho^6$  model) at temperatures above the critical value of  $T_c$  ( $T_c$  is the phase-transition temperature in the absence of an external field). The free energy of the system is found by separating the contributions from the short- and long-wave spin-density oscillation modes taking into account both the temperature and field fluctuations of the order parameter. Our analytical calculations do not involve power series in the scaling variable and are valid in the whole field-temperature plane near the critical point including the region in the vicinity of the limiting field  $\tilde{h}_c$ , which divides external fields into the weak and strong ones (i.e., the crossover region). In this region, the temperature and field effects on the system are equivalent, the scaling variable is of the order of unity, and power series are not efficient. The obtained expression for the free energy contains the leading terms and terms determining the temperature and field confluent corrections.

PACS numbers: 05.50.+q, 05.70.Ce, 64.60.Fr, 75.10.Hk

## 1 Introduction

Despite the great successes in the investigation of three-dimensional (3D) Ising-like systems made by means of various methods (see, for example, [1]), the statistical description of the critical behavior of the mentioned systems in terms of the temperature and field variables and the calculation of scaling functions are still of interest [2]. The Ising model is widely used in the theory of phase transitions for the study of the properties of various magnetic and non-magnetic systems (ferroelectrics, ferromagnets, binary mixtures, etc.).

The description of the phase transitions in the 3D magnets, usually, is associated with the absence of exact solutions and with many approximate approaches for obtaining different system characteristics. In this article, the behavior of a 3D Ising-like system near the critical point in a homogeneous external field is studied using the collective variables (CV) method [3–5]. The main peculiarity of this method is the integration of short-wave spin-density oscillation modes, which is generally done without using perturbation theory. The CV method is similar to the Wilson non-perturbative renormalization-group (RG) approach (integration on fast modes and construction of an effective theory for slow modes) [6–8]. The term collective variables is a common name for a special class of variables that are specific for each individual physical system [3, 4]. The CV set contains variables associated with order parameters. Because of this, the phase space of CV is most natural for describing a phase transition. For magnetic systems, the CV  $\rho_{\mathbf{k}}$  are the variables associated with modes of spin-moment density oscillations, while the order parameter is related to the variable  $\rho_0$ , in which the subscript “0” corresponds to the peak of the Fourier transform of the interaction potential.

The free energy of a 3D Ising-like system in an external field at temperatures above  $T_c$  is calculated using the non-Gaussian spin-density fluctuations, namely the sextic measure density. The latter is represented as an exponential function of the CV whose argument includes the powers with the corresponding coupling constants up to the sixth power of the variable (the  $\rho^6$  model).

The present publication supplements the earlier works [9–12], in which the  $\rho^6$  model was used for calculating the free energy and other thermodynamic functions of the system in the absence of an external field. The  $\rho^6$  model provides a better quantitative description of the critical behavior of a 3D Ising-like magnet than the  $\rho^4$  model [11]. For each of the  $\rho^{2m}$  models, there exists a preferred value of the RG parameter  $s = s^*$  ( $s^* = 3.5862$  for the  $\rho^4$  model,  $s^* = 2.7349$  for the  $\rho^6$  model,  $s^* = 2.6511$  for the  $\rho^8$  model, and  $s^* = 2.6108$  for the  $\rho^{10}$  model) nullifying the average value of the coefficient in the term with the second power in the effective density of measure at the fixed point. The values of  $s$  close to  $s^*$  are optimal for the given method of calculations. The difference form of the recurrence relations (RR) between the coefficients of effective non-Gaussian densities of measures operates successfully just in this region of  $s$ . It was established (see, for example, [11, 12]) that as the form of the density of measure becomes more complicated, the dependence of the critical exponent of the correlation length  $\nu$  on the RG

parameter  $s$  becomes weaker gradually, and, starting from the sextic density of measure, the value of the exponent  $\nu$ , having a tendency to saturate with increasing  $m$  (which characterizes the order of the  $\rho^{2m}$  model,  $m = 2, 3, 4, 5$ ), changes insignificantly. The Ising model corresponds to the  $\rho^{2m}$  model approximation, where the order of the model  $2m \geq 4$ . The  $\rho^4$  model allows us to go beyond the classical analysis and to describe all qualitative aspects of the second-order phase transition. The critical behavior of a 3D Ising-like system within the CV method can be described quantitatively at  $2m \geq 6$ , and, in particular, at  $2m = 6$ . It was shown in [11,13] that the graphs of the temperature dependences of the order parameter (the spontaneous magnetization) and specific heat for the  $\rho^6$  model agree more closely with the Liu and Fisher's results [14] than the corresponding plots for the  $\rho^4$  model. The correctness of the choice of the  $\rho^6$  model for investigations is also confirmed in [15] and [16], where the effective potential is studied for the scalar field theory in three dimensions in the symmetric and spontaneously broken phases, respectively. In this case, probability distributions of average magnetization in the 3D Ising model in an external field, obtained with the help of the Monte Carlo method, were used. Tsypin [15,16] proved that the term with the sixth power of the variable in the effective potential plays an important role.

The methods existing at present make it possible to calculate universal quantities to a quite high degree of accuracy (see, for example, [1]). The advantage of the CV method lies in the possibility of obtaining and analysing thermodynamic characteristics as functions of the microscopic parameters of the initial system [11–13]. The results of calculations for a 3D Ising system on the basis of the  $\rho^4$  and  $\rho^6$  models are in accord with the results obtained by other authors (see [11,13]). In [17], the scaling functions of the order parameter and susceptibility, calculated on the basis of the free energy for the  $\rho^4$  model, were graphically compared with other authors' data. Our results accord with the results obtained within the framework of the parametric representation of the equation of state [18] and Monte Carlo simulations [2].

The expressions for the thermodynamic characteristics of the system in the presence of an external field have already been obtained on the basis of the simplest non-Gaussian measure density (the  $\rho^4$  model) in [19–22] using the point of exit of the system from the critical regime as a function of the temperature (the weak-field region) or of the field (the strong-field region). In [19,20], the thermodynamic characteristics are presented in the form of series expansions in the variables, which are combinations of the tempera-

ture and field. Our calculations in the  $\rho^4$  model approximation were also performed for temperatures  $T > T_c$  [21] and  $T < T_c$  [22] without using similar expansions for the roots of cubic equations appearing in the theoretical analysis. In this article, the free energy of a 3D uniaxial magnet within the framework of the more complicated  $\rho^6$  model is found without using series expansions introducing the generalized point of exit of the system from the critical regime. This point takes into account the temperature and field variables simultaneously. In our earlier article [17], the point of exit of the system from the critical regime was found in the simpler non-Gaussian approximation (the  $\rho^4$  model) using the numerical calculations. In contrast to [17], the point of exit of the system in the present article is explicitly defined as a function of the temperature and field. This allows one to obtain the free energy without involving the numerical calculations that is our problem solved in the present article.

## 2 Integration of partition function of the system in the $\rho^6$ model approximation taking into account effect of an external field

We consider a 3D Ising-like system on a simple cubic lattice with  $N$  sites and period  $c$  in a homogeneous external field  $h$ . The Hamiltonian of such a system has the form

$$H = -\frac{1}{2} \sum_{\mathbf{j}, \mathbf{l}} \Phi(r_{\mathbf{j}\mathbf{l}}) \sigma_{\mathbf{j}} \sigma_{\mathbf{l}} - h \sum_{\mathbf{j}} \sigma_{\mathbf{j}}, \quad (1)$$

where  $r_{\mathbf{j}\mathbf{l}}$  is the distance between particles at sites  $\mathbf{j}$  and  $\mathbf{l}$ , and  $\sigma_{\mathbf{j}}$  is the operator of the  $z$  component of spin at the  $\mathbf{j}$ th site, having two eigenvalues +1 and -1. The interaction potential is an exponentially decreasing function

$$\Phi(r_{\mathbf{j}\mathbf{l}}) = A \exp\left(-\frac{r_{\mathbf{j}\mathbf{l}}}{b}\right). \quad (2)$$

Here  $A$  is a constant and  $b$  is the radius of effective interaction. For the Fourier transform of the interaction potential, we use the following approximation [3, 11, 12]:

$$\tilde{\Phi}(k) = \begin{cases} \tilde{\Phi}(0)(1 - 2b^2k^2), & k \leq B', \\ 0, & B' < k \leq B, \end{cases} \quad (3)$$

where  $B$  is the boundary of the Brillouin half-zone ( $B = \pi/c$ ),  $B' = (b\sqrt{2})^{-1}$ ,  $\tilde{\Phi}(0) = 8\pi A(b/c)^3$ .

In the CV representation for the partition function of the system, we have [3, 23]

$$Z = \int \exp \left[ \frac{1}{2} \sum_{\mathbf{k}} \beta \tilde{\Phi}(k) \rho_{\mathbf{k}} \rho_{-\mathbf{k}} + \beta h \sqrt{N} \rho_0 \right] J(\rho) (d\rho)^N. \quad (4)$$

Here the summation over the wave vectors  $\mathbf{k}$  is carried out within the first Brillouin zone,  $\beta = 1/(kT)$  is the inverse thermodynamic temperature, the CV  $\rho_{\mathbf{k}}$  are introduced by means of the functional representation for operators of spin-density oscillation modes  $\hat{\rho}_{\mathbf{k}} = (\sqrt{N})^{-1} \sum_{\mathbf{l}} \sigma_{\mathbf{l}} \exp(-i\mathbf{k}\mathbf{l})$ ,

$$\begin{aligned} J(\rho) = & 2^N \int \exp \left[ 2\pi i \sum_{\mathbf{k}} \omega_{\mathbf{k}} \rho_{\mathbf{k}} + \sum_{n \geq 1} (2\pi i)^{2n} N^{1-n} \right. \\ & \left. \times \frac{\mathcal{M}_{2n}}{(2n)!} \sum_{\mathbf{k}_1, \dots, \mathbf{k}_{2n}} \omega_{\mathbf{k}_1} \cdots \omega_{\mathbf{k}_{2n}} \delta_{\mathbf{k}_1 + \dots + \mathbf{k}_{2n}} \right] (d\omega)^N \end{aligned} \quad (5)$$

is the Jacobian of transition from the set of  $N$  spin variables  $\sigma_{\mathbf{l}}$  to the set of CV  $\rho_{\mathbf{k}}$ , and  $\delta_{\mathbf{k}_1 + \dots + \mathbf{k}_{2n}}$  is the Kronecker symbol. The variables  $\omega_{\mathbf{k}}$  are conjugate to  $\rho_{\mathbf{k}}$ , and the cumulants  $\mathcal{M}_{2n}$  assume constant values (see [3–5]).

Proceeding from Eqs. (4) and (5), we obtain the following initial expression for the partition function of the system in the  $\rho^6$  model approximation:

$$\begin{aligned} Z = & 2^N 2^{(N'-1)/2} e^{a'_0 N'} \int \exp \left[ -a'_1 (N')^{1/2} \rho_0 \right. \\ & - \frac{1}{2} \sum_{\substack{\mathbf{k} \\ k \leq B'}} d'(k) \rho_{\mathbf{k}} \rho_{-\mathbf{k}} - \sum_{l=2}^3 \frac{a'_{2l}}{(2l)! (N')^{l-1}} \\ & \left. \times \sum_{\substack{\mathbf{k}_1, \dots, \mathbf{k}_{2l} \\ k_i \leq B'}} \rho_{\mathbf{k}_1} \cdots \rho_{\mathbf{k}_{2l}} \delta_{\mathbf{k}_1 + \dots + \mathbf{k}_{2l}} \right] (d\rho)^{N'}. \end{aligned} \quad (6)$$

Here  $N' = N s_0^{-d}$  ( $d = 3$  is the space dimension),  $s_0 = B/B' = \pi\sqrt{2}b/c$ , and  $a'_1 = -s_0^{d/2} h'$ ,  $h' = \beta h$ . The expressions for the remaining coefficients are given in [9–12]. These coefficients are functions of  $s_0$ , i.e., of the ratio of microscopic parameters  $b$  and  $c$ . The integration over the zeroth, first, second,

...,  $n$ th layers of the CV phase space [3–5, 11] leads to the representation of the partition function in the form of a product of the partial partition functions  $Q_n$  of individual layers and the integral of the “smoothed” effective measure density

$$Z = 2^N 2^{(N_{n+1}-1)/2} Q_0 Q_1 \cdots Q_n [Q(P_n)]^{N_{n+1}} \times \int \mathcal{W}_6^{(n+1)}(\rho) (d\rho)^{N_{n+1}}. \quad (7)$$

The expressions for  $Q_n$ ,  $Q(P_n)$  are presented in [9–12], and  $N_{n+1} = N' s^{-d(n+1)}$ . The sextic measure density of the  $(n+1)$ th block structure  $\mathcal{W}_6^{(n+1)}(\rho)$  has the form

$$\begin{aligned} & \mathcal{W}_6^{(n+1)}(\rho) \\ &= \exp \left[ -a_1^{(n+1)} N_{n+1}^{1/2} \rho_0 - \frac{1}{2} \sum_{\mathbf{k}}_{k \leq B_{n+1}} d_{n+1}(k) \rho_{\mathbf{k}} \rho_{-\mathbf{k}} \right. \\ & \quad \left. - \sum_{l=2}^3 \frac{a_{2l}^{(n+1)}}{(2l)! N_{n+1}^{l-1}} \sum_{\substack{\mathbf{k}_1, \dots, \mathbf{k}_{2l} \\ k_i \leq B_{n+1}}} \rho_{\mathbf{k}_1} \cdots \rho_{\mathbf{k}_{2l}} \delta_{\mathbf{k}_1 + \dots + \mathbf{k}_{2l}} \right], \end{aligned} \quad (8)$$

where  $B_{n+1} = B' s^{-(n+1)}$ ,  $d_{n+1}(k) = a_2^{(n+1)} - \beta \tilde{\Phi}(k)$ ,  $a_1^{(n+1)}$  and  $a_{2l}^{(n+1)}$  are the renormalized values of the coefficients  $a'_1$  and  $a'_{2l}$  after integration over  $n+1$  layers of the phase space of CV. The coefficients  $a_1^{(n)} = s^{-n} t_n$ ,  $d_n(0) = s^{-2n} r_n$  [appearing in  $d_n(k) = d_n(0) + 2\beta \tilde{\Phi}(0) b^2 k^2$ ],  $a_4^{(n)} = s^{-4n} u_n$ , and  $a_6^{(n)} = s^{-6n} w_n$  are connected with the coefficients of the  $(n+1)$ th layer through the RR

$$\begin{aligned} t_{n+1} &= s^{(d+2)/2} t_n, \\ r_{n+1} &= s^2 \left[ -q + u_n^{1/2} Y(h_n, \alpha_n) \right], \\ u_{n+1} &= s^{4-d} u_n B(h_n, \alpha_n), \\ w_{n+1} &= s^{6-2d} u_n^{3/2} D(h_n, \alpha_n) \end{aligned} \quad (9)$$

whose solutions

$$\begin{aligned} t_n &= t^{(0)} - s_0^{d/2} h' E_1^n, \\ r_n &= r^{(0)} + c_1 E_2^n + c_2 w_{12}^{(0)} (u^{(0)})^{-1/2} E_3^n \\ & \quad + c_3 w_{13}^{(0)} (u^{(0)})^{-1} E_4^n, \end{aligned}$$

$$\begin{aligned}
u_n &= u^{(0)} + c_1 w_{21}^{(0)} (u^{(0)})^{1/2} E_2^n + c_2 E_3^n \\
&\quad + c_3 w_{23}^{(0)} (u^{(0)})^{-1/2} E_4^n, \\
w_n &= w^{(0)} + c_1 w_{31}^{(0)} u^{(0)} E_2^n \\
&\quad + c_2 w_{32}^{(0)} (u^{(0)})^{1/2} E_3^n + c_3 E_4^n
\end{aligned} \tag{10}$$

in the region of the critical regime are used for calculating the free energy of the system. Here

$$\begin{aligned}
Y(h_n, \alpha_n) &= s^{d/2} F_2(\eta_n, \xi_n) [C(h_n, \alpha_n)]^{-1/2}, \\
B(h_n, \alpha_n) &= s^{2d} C(\eta_n, \xi_n) [C(h_n, \alpha_n)]^{-1}, \\
D(h_n, \alpha_n) &= s^{7d/2} N(\eta_n, \xi_n) [C(h_n, \alpha_n)]^{-3/2}.
\end{aligned} \tag{11}$$

The quantity  $q = \bar{q} \beta \tilde{\Phi}(0)$  determines the average value of the Fourier transform of the potential  $\beta \tilde{\Phi}(B_{n+1}, B_n) = \beta \tilde{\Phi}(0) - q/s^{2n}$  in the  $n$ th layer (in this article,  $\bar{q} = (1 + s^{-2})/2$  corresponds to the arithmetic mean value of  $k^2$  on the interval  $(1/s, 1]$ ). The basic arguments  $h_n$  and  $\alpha_n$  are determined by the coefficients of the sextic measure density of the  $n$ th block structure. The intermediate variables  $\eta_n$  and  $\xi_n$  are functions of  $h_n$  and  $\alpha_n$ . The expressions for both basic and intermediate arguments as well as the special functions appearing in Eqs. (11) are the same as in the absence of an external field (see [9–12]). The quantities  $E_l$  in Eqs. (10) are the eigenvalues of the matrix of the RG linear transformation

$$\begin{pmatrix} t_{n+1} - t^{(0)} \\ r_{n+1} - r^{(0)} \\ u_{n+1} - u^{(0)} \\ w_{n+1} - w^{(0)} \end{pmatrix} = \begin{pmatrix} R_{11} & 0 & 0 & 0 \\ 0 & R_{22} & R_{23} & R_{24} \\ 0 & R_{32} & R_{33} & R_{34} \\ 0 & R_{42} & R_{43} & R_{44} \end{pmatrix} \begin{pmatrix} t_n - t^{(0)} \\ r_n - r^{(0)} \\ u_n - u^{(0)} \\ w_n - w^{(0)} \end{pmatrix}. \tag{12}$$

We have  $E_1 = R_{11} = s^{(d+2)/2}$ . Other nonzero matrix elements  $R_{ij}$  ( $i = 2, 3, 4$ ;  $j = 2, 3, 4$ ) and the eigenvalues  $E_2, E_3, E_4$  coincide, respectively, with the quantities  $R_{i_1 j_1}$  ( $i_1 = i - 1$ ;  $j_1 = j - 1$ ) and  $E_1, E_2, E_3$  obtained in the case of  $h = 0$ . The quantities  $f_0, \varphi_0$ , and  $\psi_0$  characterizing the fixed-point coordinates

$$\begin{aligned}
t^{(0)} &= 0, & r^{(0)} &= -f_0 \beta \tilde{\Phi}(0), \\
u^{(0)} &= \varphi_0 (\beta \tilde{\Phi}(0))^2, & w^{(0)} &= \psi_0 (\beta \tilde{\Phi}(0))^3
\end{aligned} \tag{13}$$

as well as the remaining coefficients in Eqs. (10) are also defined on the basis of expressions corresponding to a zero external field.

### 3 Using the generalized point of exit of the system from the critical-regime region for calculating the free energy

Let us calculate the free energy  $F = -kT \ln Z$  of a 3D Ising-like system above the critical temperature  $T_c$ . The basic idea of such a calculation on the microscopic level consists in the separate inclusion of the contributions from short-wave ( $F_{CR}$ , the region of the critical regime) and long-wave ( $F_{LGR}$ , the region of the limiting Gaussian regime) modes of spin-moment density oscillations [3–5]:

$$F = F_0 + F_{CR} + F_{LGR}. \quad (14)$$

Here  $F_0 = -kTN \ln 2$  is the free energy of  $N$  noninteracting spins. Each of three components in Eq. (14) corresponds to individual factor in the convenient representation

$$Z = 2^N Z_{CR} Z_{LGR} \quad (15)$$

for the partition function given by Eq. (7). The contributions from short- and long-wave modes to the free energy of the system in the presence of an external field are calculated in the  $\rho^6$  model approximation according to the scheme proposed in [9–12]. Short-wave modes are characterized by a RG symmetry and are described by the non-Gaussian measure density. The calculation of the contribution from long-wave modes is based on using the Gaussian measure density as the basis one. Here, we have developed a direct method of calculations with the results obtained by taking into account the short-wave modes as initial parameters. The main results obtained in the course of deriving the complete expression for the free energy of the system are presented below.

#### 3.1 Region of the critical regime

A calculation technique based on the  $\rho^6$  model for the contribution  $F_{CR}$  is similar to that elaborated in the absence of an external field (see, for example, [5, 10, 11]). Carrying out the summation of partial tree energies  $F_n$  over the layers of the phase space of CV, we can calculate  $F_{CR}$ :

$$F_{CR} = F'_0 + F'_{CR},$$



$$\begin{aligned}
F'_0 &= -kTN'[\ln Q(\mathcal{M}) + \ln Q(d)], \\
F'_{CR} &= \sum_{n=1}^{n_p} F_n.
\end{aligned} \tag{16}$$

An explicit dependence of  $F_n$  on the layer number  $n$  is obtained using solutions (10) of RR and series expansions of special functions in small deviations of the basic arguments from their values at the fixed point. The main peculiar feature of the present calculations lies in using the generalized point of exit of the system from the critical regime of order-parameter fluctuations. The inclusion of the more complicated expression for the exit point (as a function of both the temperature and field variables) [24]

$$n_p = -\frac{\ln(\tilde{h}^2 + \tilde{h}_c^2)}{2 \ln E_1} - 1 \tag{17}$$

leads to the distinction between formula (16) for  $F'_{CR}$  and the analogous relation at  $h = 0$  [10, 11]. The quantity  $\tilde{h} = h'/f_0$  is determined by the dimensionless field  $h'$ , while the quantity  $\tilde{h}_c = \tilde{\tau}^{p_0}$  is a function of the reduced temperature  $\tau = (T - T_c)/T_c$ . Here  $\tilde{\tau} = \tilde{c}_1^{(0)}\tau/f_0$ ,  $p_0 = \ln E_1/\ln E_2 = (d+2)\nu/2$ ,  $\tilde{c}_1^{(0)}$  characterizes the coefficient  $c_1$  in solutions (10) of RR,  $\nu = \ln s/\ln E_2$  is the critical exponent of the correlation length. At  $h = 0$ ,  $n_p$  becomes  $m_\tau = -\ln \tilde{\tau}/\ln E_2 - 1$  (see [5, 10, 11]). At  $T = T_c$  ( $\tau = 0$ ), the quantity  $n_p$  coincides with the exit point  $n_h = -\ln \tilde{h}/\ln E_1 - 1$  [25]. The limiting value of the field  $\tilde{h}_c$  is obtained by the equality of the exit points defined by the temperature and by the field ( $m_\tau = n_h$ ).

Having expression (17) for  $n_p$ , we arrive at the relations [26]

$$\begin{aligned}
E_1^{n_p+1} &= (\tilde{h}^2 + \tilde{h}_c^2)^{-1/2}, & \tilde{\tau} E_2^{n_p+1} &= H_c, \\
H_c &= \tilde{h}_c^{1/p_0} (\tilde{h}^2 + \tilde{h}_c^2)^{-1/(2p_0)}, \\
E_3^{n_p+1} &= H_3, & H_3 &= (\tilde{h}^2 + \tilde{h}_c^2)^{\Delta_1/(2p_0)}, \\
E_4^{n_p+1} &= H_4, & H_4 &= (\tilde{h}^2 + \tilde{h}_c^2)^{\Delta_2/(2p_0)}, \\
s^{-(n_p+1)} &= (\tilde{h}^2 + \tilde{h}_c^2)^{1/(d+2)},
\end{aligned} \tag{18}$$

where  $\Delta_1 = -\ln E_3/\ln E_2$  and  $\Delta_2 = -\ln E_4/\ln E_2$  are the exponents, which determine the first and second confluent corrections, respectively. Numerical values of the quantities  $E_l$  ( $l = 1, 2, 3, 4$ ),  $\nu$ ,  $\Delta_1$ , and  $\Delta_2$  for the optimal RG parameter  $s = s^* = 2.7349$  are given in Table 1. In the weak-field region

Table 1: The eigenvalues  $E_l$  and the exponents  $\nu$ ,  $\Delta_1$ ,  $\Delta_2$  for the  $\rho^6$  model.

$E_1$	$E_2$	$E_3$	$E_4$	$\nu$	$\Delta_1$	$\Delta_2$
12.3695	4.8468	0.4367	0.0032	0.637	0.525	3.647

( $\tilde{h} \ll \tilde{h}_c$ ), quantities (18) can be calculated with the help of the following expansions:

$$\begin{aligned}
E_1^{n_p+1} &= \tilde{h}_c^{-1} \left( 1 - \frac{1}{2} \frac{\tilde{h}^2}{\tilde{h}_c^2} \right), & \tilde{h}_c^{-1} &= \tilde{\tau}^{-p_0}, \\
H_c &= 1 - \frac{1}{2p_0} \frac{\tilde{h}^2}{\tilde{h}_c^2}, \\
H_3 &= \tilde{h}_c^{\Delta_1/p_0} \left( 1 + \frac{\Delta_1}{2p_0} \frac{\tilde{h}^2}{\tilde{h}_c^2} \right), & \tilde{h}_c^{\Delta_1/p_0} &= \tilde{\tau}^{\Delta_1}, \\
H_4 &= \tilde{h}_c^{\Delta_2/p_0} \left( 1 + \frac{\Delta_2}{2p_0} \frac{\tilde{h}^2}{\tilde{h}_c^2} \right), & \tilde{h}_c^{\Delta_2/p_0} &= \tilde{\tau}^{\Delta_2}, \\
s^{-(n_p+1)} &= \tilde{h}_c^{2/(d+2)} \left( 1 + \frac{1}{d+2} \frac{\tilde{h}^2}{\tilde{h}_c^2} \right), \\
\tilde{h}_c^{2/(d+2)} &= \tilde{\tau}^\nu.
\end{aligned} \tag{19}$$

In the strong-field region ( $\tilde{h} \gg \tilde{h}_c$ ), these quantities satisfy the expressions

$$\begin{aligned}
E_1^{n_p+1} &= \tilde{h}^{-1} \left( 1 - \frac{1}{2} \frac{\tilde{h}_c^2}{\tilde{h}^2} \right), \\
H_c &= (\tilde{h}_c/\tilde{h})^{1/p_0} \left( 1 - \frac{1}{2p_0} \frac{\tilde{h}_c^2}{\tilde{h}^2} \right), \\
H_3 &= \tilde{h}^{\Delta_1/p_0} \left( 1 + \frac{\Delta_1}{2p_0} \frac{\tilde{h}_c^2}{\tilde{h}^2} \right), \\
H_4 &= \tilde{h}^{\Delta_2/p_0} \left( 1 + \frac{\Delta_2}{2p_0} \frac{\tilde{h}_c^2}{\tilde{h}^2} \right), \\
s^{-(n_p+1)} &= \tilde{h}^{2/(d+2)} \left( 1 + \frac{1}{d+2} \frac{\tilde{h}_c^2}{\tilde{h}^2} \right).
\end{aligned} \tag{20}$$

It should be noted that the variables  $\tilde{h}/\tilde{h}_c$  (the weak fields) and  $(\tilde{h}_c/\tilde{h})^{1/p_0}$  (the strong fields) coincide with the accepted choice of the arguments for scaling functions in accordance with the scaling theory. In the particular case of  $h = 0$  and  $\tau \neq 0$ , Eqs. (19) are defined as  $E_1^{n_p+1} = \tilde{\tau}^{-p_0}$ ,  $H_c = 1$ ,  $H_3 = \tilde{\tau}^{\Delta_1}$ ,  $H_4 = \tilde{\tau}^{\Delta_2}$ ,  $s^{-(n_p+1)} = \tilde{\tau}^\nu$ . At  $h \neq 0$  and  $\tau = 0$ , we have  $\tilde{h}E_1^{n_p+1} = 1$ ,  $H_c = 0$ ,  $H_3 = \tilde{h}^{\Delta_1/p_0}$ ,  $H_4 = \tilde{h}^{\Delta_2/p_0}$ ,  $s^{-(n_p+1)} = \tilde{h}^{2/(d+2)}$  [see Eqs. (20)].

We shall perform the further calculations on the basis of Eqs. (18), which are valid in the general case for the regions of small, intermediate (the crossover region), and large field values. The inclusion of  $E_3^{n_p+1}$  (or  $H_3$ ) leads to the formation of the first confluent corrections in the expressions for thermodynamic characteristics of the system. The quantity  $E_4^{n_p+1}$  (or  $H_4$ ) is responsible for the emergence of the second confluent corrections. The cases of the weak or strong fields can be obtained from general expressions by using Eqs. (19) or (20). We disregard the second confluent correction in our calculations. This is due to the fact that the contribution from the first confluent correction to thermodynamic functions near the critical point ( $\tau = 0$ ,  $h = 0$ ) for various values of  $s$  is more significant than the small contribution from the second correction ( $\tilde{h}^2 + \tilde{h}_c^2 \ll 1$ ,  $\Delta_1$  is of the order of 0.5, and  $\Delta_2 > 2$ , see Table 1 and [9]).

Proceeding from an explicit dependence of  $F_n$  on the layer number  $n$  [5, 9, 10] and taking into account Eqs. (18), we can now write the final expression for  $F_{CR}$  (16):

$$\begin{aligned} F_{CR} &= -kTN' \left( \gamma_0^{(CR)} + \gamma_1\tau + \gamma_2\tau^2 \right) + F_s, \\ F_s &= kTN' s^{-3(n_p+1)} \left( \bar{\gamma}_3^{(CR)(0)+} + \bar{\gamma}_3^{(CR)(1)+} c_{20}^{(0)} H_3 \right). \end{aligned} \quad (21)$$

Here  $c_{20}^{(0)}$  characterizes  $c_2$  in solutions (10) of RR,

$$\begin{aligned} \bar{\gamma}_3^{(CR)(0)+} &= \frac{f_{CR}^{(0)}}{1-s^{-3}} + \frac{f_{CR}^{(1)} \varphi_0^{-1/2} f_0 H_c}{1-E_2 s^{-3}} \\ &\quad + \frac{f_{CR}^{(7)} \varphi_0^{-1} (f_0 H_c)^2}{1-E_2^2 s^{-3}}, \\ \bar{\gamma}_3^{(CR)(1)+} &= \frac{f_{CR}^{(2)} \varphi_0^{-1}}{1-E_3 s^{-3}} + \frac{f_{CR}^{(4)} \varphi_0^{-3/2} f_0 H_c}{1-E_2 E_3 s^{-3}} \\ &\quad + \frac{f_{CR}^{(8)} \varphi_0^{-2} (f_0 H_c)^2}{1-E_2^2 E_3 s^{-3}}, \end{aligned} \quad (22)$$

and the coefficients

$$\begin{aligned}\gamma_0^{(CR)} &= \gamma_0^{(0)} + \delta_0^{(0)}, \\ \gamma_k &= \gamma_0^{(k)} + \delta_0^{(k)}, \quad k = 1, 2\end{aligned}\tag{23}$$

are determined by the components of the quantities

$$\begin{aligned}\gamma_0 &= \gamma_0^{(0)} + \gamma_0^{(1)}\tau + \gamma_0^{(2)}\tau^2, \\ \delta_0 &= \delta_0^{(0)} + \delta_0^{(1)}\tau + \delta_0^{(2)}\tau^2.\end{aligned}\tag{24}$$

The components  $\delta_0^{(i)}$  ( $i = 0, 1, 2$ ) satisfy the earlier relations [5, 9, 10] obtained in the case of a zero external field. The components  $\gamma_0^{(i)}$  are given by the corresponding expressions at  $h = 0$  under condition that the eigenvalues  $E_1$ ,  $E_2$ , and  $E_3$  should be replaced by  $E_2$ ,  $E_3$ , and  $E_4$ , respectively.

Let us now calculate the contribution to the free energy of the system from the layers of the CV phase space beyond the point of exit from the critical-regime region. The calculations are performed according to the scheme proposed in [3, 5, 11, 12]. As in the previous study, while calculating the partition function component  $Z_{LGR}$  from Eq. (15), it is convenient to single out two regions of values of wave vectors. The first is the transition region ( $Z_{LGR}^{(1)}$ ) corresponding to values of  $\mathbf{k}$  close to  $B_{n_p}$ , while the second is the Gaussian region ( $Z_{LGR}^{(2)}$ ) corresponding to small values of wave vector ( $k \rightarrow 0$ ). Thus, we have

$$Z_{LGR} = Z_{LGR}^{(1)} Z_{LGR}^{(2)}.\tag{25}$$

### 3.2 Transition region

This region corresponds to  $\tilde{m}_0$  layers of the phase space of CV. The lower boundary of the transition region is determined by the point of exit of the system from the critical-regime region ( $n = n_p + 1$ ). The upper boundary corresponds to the layer  $n_p + \tilde{m}_0 + 1$ . We use for  $\tilde{m}_0$  the integer closest to  $\tilde{m}'_0$ . The condition for obtaining  $\tilde{m}'_0$  is the equality [10, 11]

$$|h_{n_p + \tilde{m}'_0}| = \frac{A_0}{1 - s^{-3}},\tag{26}$$

where  $A_0$  is a large number ( $A_0 \geq 10$ ).

The free energy contribution

$$\begin{aligned}
F_{LGR}^{(1)} &= -kTN_{n_p+1} \sum_{m=0}^{\tilde{m}_0} s^{-3m} f_{LGR_1}(m), \\
f_{LGR_1}(m) &= \ln\left(\frac{2}{\pi}\right) + \frac{1}{4} \ln 24 - \frac{1}{4} \ln C(\eta_{n_p+m}, \xi_{n_p+m}) \\
&\quad + \ln I_0(h_{n_p+m+1}, \alpha_{n_p+m+1}) \\
&\quad + \ln I_0(\eta_{n_p+m}, \xi_{n_p+m})
\end{aligned} \tag{27}$$

corresponding to  $Z_{LGR}^{(1)}$  from Eq. (25) is calculated by using the solutions of RR.

The basic arguments in the  $(n_p + m)$ th layer

$$\begin{aligned}
h_{n_p+m} &= (r_{n_p+m} + q)(6/u_{n_p+m})^{1/2}, \\
\alpha_{n_p+m} &= \frac{\sqrt{6}}{15} w_{n_p+m}/u_{n_p+m}^{3/2}
\end{aligned} \tag{28}$$

can be presented using the relations

$$\begin{aligned}
t_{n_p+m} &= -s_0^{d/2} f_0 E_1^{m-1} \tilde{h}(\tilde{h}^2 + \tilde{h}_c^2)^{-1/2}, \\
r_{n_p+m} &= \beta \tilde{\Phi}(0) \left( -f_0 + f_0 H_c E_2^{m-1} \right. \\
&\quad \left. + c_{20}^{(0)} H_3 \varphi_0^{-1/2} w_{12}^{(0)} E_3^{m-1} \right), \\
u_{n_p+m} &= (\beta \tilde{\Phi}(0))^2 \left( \varphi_0 + f_0 H_c \varphi_0^{1/2} w_{21}^{(0)} E_2^{m-1} \right. \\
&\quad \left. + c_{20}^{(0)} H_3 E_3^{m-1} \right), \\
w_{n_p+m} &= (\beta \tilde{\Phi}(0))^3 \left( \psi_0 + f_0 H_c \varphi_0 w_{31}^{(0)} E_2^{m-1} \right. \\
&\quad \left. + c_{20}^{(0)} H_3 \varphi_0^{1/2} w_{32}^{(0)} E_3^{m-1} \right)
\end{aligned} \tag{29}$$

obtained on the basis of Eqs. (10) and (18). We arrive at the following expressions:

$$\begin{aligned}
h_{n_p+m} &= h_{n_p+m}^{(0)} \left( 1 + \bar{h}_{n_p+m}^{(1)} c_{20}^{(0)} H_3 \right), \\
h_{n_p+m}^{(0)} &= \sqrt{6} \frac{\bar{q} - f_0 + f_0 H_c E_2^{m-1}}{(\varphi_0 + f_0 H_c \varphi_0^{1/2} w_{21}^{(0)} E_2^{m-1})^{1/2}}, \\
\bar{h}_{n_p+m}^{(1)} &= E_3^{m-1} \left( \frac{\varphi_0^{-1/2} w_{12}^{(0)}}{\bar{q} - f_0 + f_0 H_c E_2^{m-1}} \right)
\end{aligned}$$

$$\begin{aligned}
& -\frac{1}{2} \frac{1}{\varphi_0 + f_0 H_c \varphi_0^{1/2} w_{21}^{(0)} E_2^{m-1}} \Big); \\
\alpha_{n_p+m} &= \alpha_{n_p+m}^{(0)} \left( 1 + \bar{\alpha}_{n_p+m}^{(1)} c_{20}^{(0)} H_3 \right), \\
\alpha_{n_p+m}^{(0)} &= \frac{\sqrt{6}}{15} \frac{\psi_0 + f_0 H_c \varphi_0 w_{31}^{(0)} E_2^{m-1}}{(\varphi_0 + f_0 H_c \varphi_0^{1/2} w_{21}^{(0)} E_2^{m-1})^{3/2}}, \\
\bar{\alpha}_{n_p+m}^{(1)} &= E_3^{m-1} \left( \frac{\varphi_0^{1/2} w_{32}^{(0)}}{\psi_0 + f_0 H_c \varphi_0 w_{31}^{(0)} E_2^{m-1}} \right. \\
& \quad \left. - \frac{3}{2} \frac{1}{\varphi_0 + f_0 H_c \varphi_0^{1/2} w_{21}^{(0)} E_2^{m-1}} \right). \tag{30}
\end{aligned}$$

In contrast to  $H_c$ , the quantity  $H_3$  in expressions (30) for  $h_{n_p+m}$  and  $\alpha_{n_p+m}$  as well as in expression (21) for  $F_s$  takes on small values with the variation of the field  $\tilde{h}$  (see Fig. 1). The quantity  $H_c$  at  $\tilde{h} \rightarrow 0$  and near  $\tilde{h}_c$  is close to

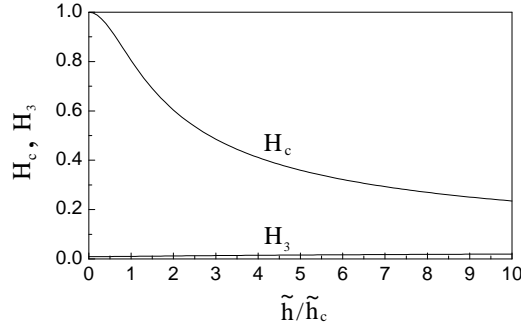


Figure 1: Dependence of quantities  $H_c$  and  $H_3$  on the ratio  $\tilde{h}/\tilde{h}_c$  for the RG parameter  $s = s^* = 2.7349$  and the reduced temperature  $\tau = 10^{-4}$ .

unity and series expansions in  $H_c$  are not effective here.

Power series in small deviations  $(h_{n_p+m} - h_{n_p+m}^{(0)})$  and  $(\alpha_{n_p+m} - \alpha_{n_p+m}^{(0)})$  for the special functions appearing in the expressions for the intermediate arguments

$$\begin{aligned}
\eta_{n_p+m} &= (6s^d)^{1/2} F_2(h_{n_p+m}, \alpha_{n_p+m}) \\
&\quad \times \left[ C(h_{n_p+m}, \alpha_{n_p+m}) \right]^{-1/2}, \\
\xi_{n_p+m} &= \frac{\sqrt{6}}{15} s^{-d/2} N(h_{n_p+m}, \alpha_{n_p+m}) \\
&\quad \times \left[ C(h_{n_p+m}, \alpha_{n_p+m}) \right]^{-3/2} \tag{31}
\end{aligned}$$

allow us to find the relations

$$\begin{aligned}
\eta_{n_p+m} &= \eta_{n_p+m}^{(0)} \left[ 1 - \left( \bar{\eta}_1^{(n_p+m)} h_{n_p+m}^{(0)} \bar{h}_{n_p+m}^{(1)} \right. \right. \\
&\quad \left. \left. + \bar{\eta}_2^{(n_p+m)} \alpha_{n_p+m}^{(0)} \bar{\alpha}_{n_p+m}^{(1)} \right) c_{20}^{(0)} H_3 \right], \\
\xi_{n_p+m} &= \xi_{n_p+m}^{(0)} \left[ 1 - \left( \bar{\xi}_1^{(n_p+m)} h_{n_p+m}^{(0)} \bar{h}_{n_p+m}^{(1)} \right. \right. \\
&\quad \left. \left. + \bar{\xi}_2^{(n_p+m)} \alpha_{n_p+m}^{(0)} \bar{\alpha}_{n_p+m}^{(1)} \right) c_{20}^{(0)} H_3 \right].
\end{aligned} \tag{32}$$

The quantities  $\eta_{n_p+m}^{(0)}$ ,  $\bar{\eta}_1^{(n_p+m)}$ ,  $\bar{\eta}_2^{(n_p+m)}$  and  $\xi_{n_p+m}^{(0)}$ ,  $\bar{\xi}_1^{(n_p+m)}$ ,  $\bar{\xi}_2^{(n_p+m)}$  are functions of  $F_{2l}^{*(n_p+m)} = I_{2l}^{*(n_p+m)} / I_0^{*(n_p+m)}$ , where

$$I_{2l}^{*(n_p+m)} = \int_0^\infty x^{2l} \exp(-h_{n_p+m}^{(0)} x^2 - x^4 - \alpha_{n_p+m}^{(0)} x^6) dx. \tag{33}$$

Proceeding from expression (27) for  $f_{LGR_1}(m)$ , we can now write the following relation accurate to within  $H_3$ :

$$\begin{aligned}
f_{LGR_1}(m) &= f_{LGR_1}^{(0)}(m) + \bar{f}_{LGR_1}^{(1)}(m) c_{20}^{(0)} H_3, \\
f_{LGR_1}^{(0)}(m) &= \ln \left( \frac{2}{\pi} \right) + \frac{1}{4} \ln 24 - \frac{1}{4} \ln C(\eta_{n_p+m}^{(0)}, \xi_{n_p+m}^{(0)}) \\
&\quad + \ln I_0(h_{n_p+m+1}^{(0)}, \alpha_{n_p+m+1}^{(0)}) \\
&\quad + \ln I_0(\eta_{n_p+m}^{(0)}, \xi_{n_p+m}^{(0)}), \\
\bar{f}_{LGR_1}^{(1)}(m) &= \varphi_1^{(n_p+m)} h_{n_p+m}^{(0)} \bar{h}_{n_p+m}^{(1)} \\
&\quad + \varphi_2^{(n_p+m)} \alpha_{n_p+m}^{(0)} \bar{\alpha}_{n_p+m}^{(1)} \\
&\quad + \varphi_3^{(n_p+m+1)} h_{n_p+m+1}^{(0)} \bar{h}_{n_p+m+1}^{(1)} \\
&\quad + \varphi_4^{(n_p+m+1)} \alpha_{n_p+m+1}^{(0)} \bar{\alpha}_{n_p+m+1}^{(1)}, \\
\varphi_k^{(n_p+m)} &= b_k^{(n_p+m)} + P_{4k}^{(n_p+m)} / 4, \quad k = 1, 2, \\
\varphi_3^{(n_p+m+1)} &= -F_2^{*(n_p+m+1)}, \\
\varphi_4^{(n_p+m+1)} &= -F_6^{*(n_p+m+1)}.
\end{aligned} \tag{34}$$

The quantities  $b_k^{(n_p+m)}$ ,  $P_{4k}^{(n_p+m)}$  depend on  $F_{2l}^{*(n_p+m)}$  as well as on  $F_{2l}^{**(n_p+m)} = I_{2l}^{**(n_p+m)} / I_0^{**(n_p+m)}$ , where

$$I_{2l}^{**(n_p+m)} = \int_0^\infty x^{2l} \exp(-\eta_{n_p+m}^{(0)} x^2 - x^4 - \xi_{n_p+m}^{(0)} x^6) dx. \tag{35}$$

The final result for  $F_{LGR}^{(1)}$  [see Eqs. (27) and (34)] assumes the form

$$\begin{aligned}
F_{LGR}^{(1)} &= -kTN's^{-3(n_p+1)} \left( \bar{f}_{TR}^{(0)} + \bar{f}_{TR}^{(1)} c_{20}^{(0)} H_3 \right), \\
\bar{f}_{TR}^{(0)} &= \sum_{m=0}^{\tilde{m}_0} s^{-3m} f_{LGR_1}^{(0)}(m), \\
\bar{f}_{TR}^{(1)} &= \sum_{m=0}^{\tilde{m}_0} s^{-3m} \bar{f}_{LGR_1}^{(1)}(m).
\end{aligned} \tag{36}$$

On the basis of Eqs. (26) and (30), it is possible to obtain the quantity  $\tilde{m}'_0$  determining the summation limit  $\tilde{m}_0$  in formulas (36):

$$\begin{aligned}
\tilde{m}'_0 &= \frac{\ln L_0 - \ln H_c}{\ln E_2} + 1, \\
L_0 &= A_1 + (A_1^2 - A_2)^{1/2}, \\
A_1 &= 1 - \frac{\bar{q}}{f_0} + \frac{A_0^2 \varphi_0^{1/2} w_{21}^{(0)}}{12 f_0 (1 - s^{-3})^2}, \\
A_2 &= 1 - 2 \frac{\bar{q}}{f_0} + \left( \frac{\bar{q}}{f_0} \right)^2 - \frac{A_0^2 \varphi_0}{6 f_0^2 (1 - s^{-3})^2}.
\end{aligned} \tag{37}$$

Let us now calculate the contribution to the free energy of the system from long-wave modes in the range of wave vectors

$$\begin{aligned}
k &\leq B' s^{-n'_p}, \\
n'_p &= n_p + \tilde{m}_0 + 2
\end{aligned} \tag{38}$$

using the Gaussian measure density.

### 3.3 Region of small values of wave vector ( $k \rightarrow 0$ )

The free energy component

$$F_{LGR}^{(2)} = \frac{1}{2} kT \left[ N_{n'_p} \ln P_2^{(n'_p-1)} + \sum_{k=0}^{B_{n'_p}} \ln \tilde{d}_{n'_p}(k) - \frac{N(h')^2}{\tilde{d}_{n'_p}(0)} \right] \tag{39}$$

corresponding to  $Z_{LGR}^{(2)}$  from Eq. (25) is similar to that presented in [5, 10, 11]. The calculations of the first and second terms in Eq. (39) are associated with



the calculations of the quantities

$$\begin{aligned}
P_2^{(n'_p-1)} &= 2h_{n'_p-1}F_2(h_{n'_p-1}, \alpha_{n'_p-1}) \\
&\quad \times \left[ d_{n'_p-1}(B_{n'_p}, B_{n'_p-1}) \right]^{-1}, \\
\tilde{d}_{n'_p}(k) &= \left[ P_2^{(n'_p-1)} \right]^{-1} + \beta \tilde{\Phi}(B_{n'_p}, B_{n'_p-1}) - \beta \tilde{\Phi}(k),
\end{aligned} \tag{40}$$

where

$$d_{n'_p-1}(B_{n'_p}, B_{n'_p-1}) = s^{-2(n'_p-1)}(r_{n'_p-1} + q), \tag{41}$$

and  $r_{n'_p-1}, h_{n'_p-1} = h_{n'_p-1}^{(0)} \left( 1 + \bar{h}_{n'_p-1}^{(1)} c_{20}^{(0)} H_3 \right)$ ,  $\alpha_{n'_p-1} = \alpha_{n'_p-1}^{(0)} \left( 1 + \bar{\alpha}_{n'_p-1}^{(1)} c_{20}^{(0)} H_3 \right)$  satisfy the corresponding expressions from Eqs. (29) and (30) at  $m = \tilde{m}_0 + 1$ .

Introducing the designation

$$p = h_{n'_p-1}F_2(h_{n'_p-1}, \alpha_{n'_p-1}) \tag{42}$$

and presenting it in the form

$$p^{-1} = p_0(1 + \bar{p}_1 c_{20}^{(0)} H_3), \tag{43}$$

we obtain the following relations for the coefficients:

$$\begin{aligned}
p_0 &= \left[ h_{n'_p-1}^{(0)} p_{20}^{(n'_p-1)} \right]^{-1}, \\
\bar{p}_1 &= -\bar{h}_{n'_p-1}^{(1)} \left( 1 - p_{21}^{(n'_p-1)} h_{n'_p-1}^{(0)} \right) \\
&\quad + p_{22}^{(n'_p-1)} \alpha_{n'_p-1}^{(0)} \bar{\alpha}_{n'_p-1}^{(1)}.
\end{aligned} \tag{44}$$

The quantities

$$\begin{aligned}
p_{20}^{(n'_p-1)} &= F_2^{*(n'_p-1)}, \quad p_{21}^{(n'_p-1)} = \frac{F_4^{*(n'_p-1)}}{F_2^{*(n'_p-1)}} - F_2^{*(n'_p-1)}, \\
p_{22}^{(n'_p-1)} &= \frac{F_8^{*(n'_p-1)}}{F_2^{*(n'_p-1)}} - F_6^{*(n'_p-1)}
\end{aligned} \tag{45}$$

determine the function

$$\begin{aligned}
F_2(h_{n'_p-1}, \alpha_{n'_p-1}) &= p_{20}^{(n'_p-1)} \left[ 1 - \left( p_{21}^{(n'_p-1)} h_{n'_p-1}^{(0)} \bar{h}_{n'_p-1}^{(1)} \right. \right. \\
&\quad \left. \left. + p_{22}^{(n'_p-1)} \alpha_{n'_p-1}^{(0)} \bar{\alpha}_{n'_p-1}^{(1)} \right) c_{20}^{(0)} H_3 \right].
\end{aligned} \tag{46}$$

Here  $F_{2l}^{*(n'_p-1)} = I_{2l}^{*(n'_p-1)} / I_0^{*(n'_p-1)}$ , where

$$I_{2l}^{*(n'_p-1)} = \int_0^\infty x^{2l} \exp(-h_{n'_p-1}^{(0)} x^2 - x^4 - \alpha_{n'_p-1}^{(0)} x^6) dx. \quad (47)$$

Taking into account Eqs. (41) and (43), we rewrite formulas (40) as

$$\begin{aligned} P_2^{(n'_p-1)} &= \left\{ \frac{1}{2} s^{-2(n'_p-1)} \beta \tilde{\Phi}(0) p_0 (\bar{q} - f_0 + f_0 H_c E_2^{\tilde{m}_0}) \right. \\ &\quad \times \left[ 1 + \left( \frac{\varphi_0^{-1/2} w_{12}^{(0)} E_3^{\tilde{m}_0}}{\bar{q} - f_0 + f_0 H_c E_2^{\tilde{m}_0}} + \bar{p}_1 \right) c_{20}^{(0)} H_3 \right] \Big\}^{-1}, \\ \tilde{d}_{n'_p}(k) &= s^{-2(n'_p-1)} \beta \tilde{\Phi}(0) \tilde{G} + 2\beta \tilde{\Phi}(0) b^2 k^2, \\ \tilde{G} &= g_0 (1 + \bar{g}_1 c_{20}^{(0)} H_3), \\ g_0 &= \frac{1}{2} \left[ (-f_0 + f_0 H_c E_2^{\tilde{m}_0}) p_0 + (p_0 - 2) \bar{q} \right], \\ \bar{g}_1 &= \frac{1}{2} \frac{p_0}{g_0} [\bar{p}_1 (\bar{q} - f_0 + f_0 H_c E_2^{\tilde{m}_0}) \\ &\quad + \varphi_0^{-1/2} w_{12}^{(0)} E_3^{\tilde{m}_0}]. \end{aligned} \quad (48)$$

The second term in Eq. (39) is defined by the expression

$$\begin{aligned} \frac{1}{2} \sum_{k=0}^{B_{n'_p}} \ln \tilde{d}_{n'_p}(k) &= N_{n'_p} \left\{ \frac{1}{2} \ln(\tilde{G} + s^{-2}) + \ln s - n'_p \ln s \right. \\ &\quad + \frac{1}{2} \ln(\beta \tilde{\Phi}(0)) - \frac{1}{3} + \tilde{G} s^2 \\ &\quad \left. - (\tilde{G} s^2)^{3/2} \arctan [(\tilde{G} s^2)^{-1/2}] \right\}. \end{aligned} \quad (49)$$

Relations (48) and (49) make it possible to find the component  $F_{LGR}^{(2)}$  in the form

$$\begin{aligned} F_{LGR}^{(2)} &= -kT \left[ N' s^{-3(n_p+1)} (\bar{f}^{(0)'} + \bar{f}^{(1)'} c_{20}^{(0)} H_3) \right. \\ &\quad \left. + \frac{N(h')^2 \bar{\gamma}_4^+}{\beta \tilde{\Phi}(0)} s^{2(n_p+1)} (1 - \bar{g}_1 c_{20}^{(0)} H_3) \right], \\ \bar{f}^{(0)'} &= s^{-3(\tilde{m}_0+1)} f^{(0)}, \quad \bar{f}^{(1)'} = s^{-3(\tilde{m}_0+1)} \bar{f}^{(1)}, \end{aligned}$$

$$\begin{aligned}
f^{(0)} &= -\frac{1}{2} \ln \left( \frac{s^{-2} + g_0}{g_0 + \bar{q}} \right) + \frac{1}{3} \\
&\quad - g'_0 \left[ 1 - \sqrt{g'_0} \arctan \left( \frac{1}{\sqrt{g'_0}} \right) \right], \\
\bar{f}^{(1)} &= \frac{1}{2} \left( \frac{g_0 \bar{g}_1}{g_0 + \bar{q}} - \frac{\bar{g}_1}{(g'_0)^{-1} + 1} - \frac{g'_0 \bar{g}_1}{(g'_0)^{-1} + 1} \right) \\
&\quad - g'_0 \bar{g}_1 \left[ 1 - \frac{3}{2} \sqrt{g'_0} \arctan \left( \frac{1}{\sqrt{g'_0}} \right) \right], \\
g'_0 &= s^2 g_0, \quad \bar{\gamma}_4^+ = s^{2\tilde{m}_0} / (2g_0).
\end{aligned} \tag{50}$$

On the basis of Eqs. (36) and (50), we can write the following expression for the general contribution  $F_{LGR} = F_{LGR}^{(1)} + F_{LGR}^{(2)}$  to the free energy of the system from long-wave modes of spin-moment density oscillations:

$$\begin{aligned}
F_{LGR} &= -kT \left[ N' s^{-3(n_p+1)} (\bar{f}_{LGR}^{(0)} + \bar{f}_{LGR}^{(1)} c_{20}^{(0)} H_3) \right. \\
&\quad \left. + \frac{N(h')^2 \bar{\gamma}_4^+}{\beta \tilde{\Phi}(0)} s^{2(n_p+1)} (1 - \bar{g}_1 c_{20}^{(0)} H_3) \right], \\
\bar{f}_{LGR}^{(l)} &= \bar{f}_{TR}^{(l)} + \bar{f}^{(l)'}, \quad l = 0, 1.
\end{aligned} \tag{51}$$

## 4 Total free energy of the system at $T > T_c$ as function of temperature, field and microscopic parameters

The total free energy of the system is calculated taking into account Eqs. (14), (21), and (51). Collecting the contributions to the free energy from all regimes of fluctuations at  $T > T_c$  in the presence of an external field and using the relation for  $s^{-(n_p+1)}$  from Eqs. (18), we obtain

$$\begin{aligned}
F &= -kTN \left[ \gamma'_0 + \gamma'_1 \tau + \gamma'_2 \tau^2 + (\bar{\gamma}_3^{(0)+} + \bar{\gamma}_3^{(1)+} c_{20}^{(0)} H_3) \right. \\
&\quad \left. \times (\tilde{h}^2 + \tilde{h}_c^2)^{3/5} + \frac{\bar{\gamma}_4^+ (h')^2}{\beta \tilde{\Phi}(0)} (1 - \bar{g}_1 c_{20}^{(0)} H_3) (\tilde{h}^2 + \tilde{h}_c^2)^{-2/5} \right], \\
\gamma'_0 &= \ln 2 + s_0^{-3} \gamma_0^{(CR)}, \quad \gamma'_1 = s_0^{-3} \gamma_1, \quad \gamma'_2 = s_0^{-3} \gamma_2,
\end{aligned}$$

$$\bar{\gamma}_3^{(l)+} = s_0^{-3}(-\bar{\gamma}_3^{(CR)(l)+} + \bar{f}_{LGR}^{(l)}), \quad l = 0, 1. \quad (52)$$

The coefficients  $\gamma_0^{(CR)}$ ,  $\gamma_1$ ,  $\gamma_2$  are defined by Eqs. (23),  $\bar{g}_1$  is presented in Eqs. (48), and  $\bar{\gamma}_4^+$  is given in Eqs. (50). The coefficients of the non-analytic component of the free energy  $F$  [see Eqs. (52)] depend on  $H_c$ . The terms proportional to  $H_3$  determine the confluent corrections by the temperature and field. As is seen from the expression for  $F$ , the free energy of the system at  $\tilde{h} = 0$  and  $\tilde{\tau} = 0$ , in addition to terms proportional to  $\tilde{\tau}^{3\nu}$  (or  $\tilde{h}_c^{6/5}$ ) and  $\tilde{h}^{6/5}$ , contains the terms proportional to  $\tilde{\tau}^{3\nu+\Delta_1}$  and  $\tilde{h}^{6/5+\Delta_1/p_0}$ , respectively. At  $\tilde{h} \neq 0$  and  $\tilde{\tau} \neq 0$ , the terms of both types are present. It should be noted that  $\Delta_1 > \Delta_1/p_0$ . At  $\tilde{h} = \tilde{h}_c$ , we have  $\tilde{\tau}^{\Delta_1} = \tilde{h}^{\Delta_1/p_0}$  and the contributions to the thermodynamic characteristics of the system from both types of the corrections become of the same order.

The advantage of the method presented in this article is the possibility of deriving analytic expressions for the free-energy coefficients as functions of the microscopic parameters of the system (the lattice constant  $c$  and parameters of the interaction potential, i.e., the effective radius  $b$  of the potential, the Fourier transform  $\tilde{\Phi}(0)$  of the potential for  $k = 0$ ).

## 5 Conclusions

An analytic method for calculating the total free energy of a 3D Ising-like system (a 3D uniaxial magnet) near the critical point is developed on the microscopic level in the higher non-Gaussian approximation based on the sextic distribution for modes of spin-moment density oscillations (the  $\rho^6$  model). The simultaneous effect of the temperature and field on the behavior of the system is taken into account. An external field is introduced in the Hamiltonian of the system from the outset. In contrast to previous studies on the basis of the asymmetric  $\rho^4$  model [19, 20, 27], the field in the initial process of calculating the partition function of the system is not included in the Jacobian of transition from the set of spin variables to the set of CV. Such an approach leads to the appearance of the first, second, fourth, and sixth powers of CV in the expression for the partition function and allows us to simplify the mathematical description because the odd part is represented only by the linear term.

The theory is being built ab initio beginning from the Hamiltonian of the system up to the expression for the free energy. The main distinctive feature

of the proposed method is the separate inclusion of the contributions to the free energy from the short- and long-wave spin-density oscillation modes. The generalized point of exit of the system from the critical regime contains both the temperature and field variables. The form of the temperature and field dependences for the free energy of the system is determined by solutions of RR near the fixed point. The expression for the free energy  $F$  obtained at temperatures  $T > T_c$  without using power series in the scaling variable and without any adjustable parameters can be employed in the field region near  $\tilde{h}_c$  (the crossover region). The limiting field  $\tilde{h}_c$  satisfies the condition of the equality of sizes of the critical-regime region by the temperature and field (the effect of the temperature and field on the system in the vicinity of the critical point is equivalent) [19, 20, 25, 27]. In the vicinity of  $\tilde{h}_c$ , the scaling variable is of the order of unity and power series in this variable are not effective. We hope that the proposed method as well as our explicit representations may provide useful benchmarks in studying the effect of an external magnetic field on the critical behavior of 3D Ising-like systems within the framework of the higher non-Gaussian approximation (the  $\rho^6$  model). Proceeding from the expression for the free energy, which involves the leading terms and terms determining the temperature and field confluent corrections, we can find other thermodynamic characteristics (the average spin moment, susceptibility, entropy, and specific heat) by direct differentiation of  $F$  with respect to field or temperature.

## References

- [1] A. Pelissetto and E. Vicari, Phys. Rep. **368**, 549 (2002).
- [2] J. Engels, L. Fromme, and M. Seniuch, Nucl. Phys. B **655** [FS], 277 (2003).
- [3] I. R. Yukhnovskii, *Phase Transitions of the Second Order. Collective Variables Method* (World Scientific, Singapore, 1987).
- [4] I. R. Yukhnovskii, Riv. Nuovo Cimento **12**, 1 (1989).
- [5] I. R. Yukhnovskii, M. P. Kozlovskii, and I. V. Pylyuk, *Microscopic Theory of Phase Transitions in the Three-Dimensional Systems* (Eurosvit, Lviv, 2001) [in Ukrainian].

- [6] J. Berges, N. Tetradis, and C. Wetterich, Phys. Rep. **363**, 223 (2002).
- [7] N. Tetradis and C. Wetterich, Nucl. Phys. B **422** [FS], 541 (1994).
- [8] C. Bagnuls and C. Bervillier, Phys. Rep. **348**, 91 (2001).
- [9] M. P. Kozlovskii, I. V. Pylyuk, and V. V. Dukhovii, Condens. Matter Phys. **11**, 17 (1997).
- [10] I. V. Pylyuk, Low Temp. Phys. **25**, 877 (1999).
- [11] I. R. Yukhnovskii, M. P. Kozlovskii, and I. V. Pylyuk, Phys. Rev. B **66**, 134410 (2002).
- [12] I. R. Yukhnovskii, I. V. Pylyuk, and M. P. Kozlovskii, J. Phys.: Condens. Matter **14**, 10113 (2002).
- [13] I. R. Yukhnovskii, I. V. Pylyuk, and M. P. Kozlovskii, J. Phys.: Condens. Matter **14**, 11701 (2002).
- [14] A. J. Liu and M. E. Fisher, Physica A **156**, 35 (1989).
- [15] M. M. Tsypin, Phys. Rev. Lett. **73**, 2015 (1994).
- [16] M. M. Tsypin, Phys. Rev. B **55**, 8911 (1997).
- [17] M. P. Kozlovskii, I. V. Pylyuk, and O. O. Prytula, Nucl. Phys. B **753** [FS], 242 (2006).
- [18] R. Guida and J. Zinn-Justin, Nucl. Phys. B **489** [FS], 626 (1997).
- [19] I. V. Pylyuk, M. P. Kozlovskii, and O. O. Prytula, Ferroelectrics **317**, 43 (2005).
- [20] M. P. Kozlovskii, I. V. Pylyuk, and O. O. Prytula, Phys. Rev. B **73**, 174406 (2006).
- [21] M. P. Kozlovskii, I. V. Pylyuk, and O. O. Prytula, Physica A **369**, 562 (2006).
- [22] M. P. Kozlovskii, I. V. Pylyuk, and O. O. Prytula, Condens. Matter Phys. **8**, 749 (2005).

- [23] V. V. Dukhovii, M. P. Kozlovskii, and I. V. Pylyuk, Theor. Math. Phys. **107**, 650 (1996).
- [24] M. P. Kozlovskii, Phase Transitions **80**, 3 (2007).
- [25] M. P. Kozlovskii, I. V. Pylyuk, and O. O. Prytula, Condens. Matter Phys. **7**, 361 (2004).
- [26] I. V. Pylyuk, Phase Transitions **80**, 11 (2007).
- [27] I. V. Pylyuk, J. Magn. Magn. Mater. **305**, 216 (2006).